

Off-diagonal terms in symmetric operators ^{*} [†]

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In this paper we provide a quantitative comparison of two obstructions for a given symmetric operator S with dense domain in Hilbert space \mathcal{H} to be selfadjoint. The first one is the pair of deficiency spaces of von Neumann, and the second one is of more recent vintage: Let P be a projection in \mathcal{H} . We say that it is *smooth* relative to S if its range is contained in the domain of S . We say that smooth projections $\{P_i\}_{i=1}^\infty$ *diagonalize* S if

- (a) $(I - P_i)SP_i = 0$ for all i , and
- (b) $\sup_i P_i = I$.

If such projections exist, then S has a selfadjoint closure (i.e., \bar{S} has a spectral resolution), and so our second obstruction to selfadjointness is defined from smooth projections P_i with $(I - P_i)SP_i \neq 0$. We prove results both in the case of a single operator S and a system of operators.

I. INTRODUCTION

The following infinite-by-infinite matrices, also called infinite tridiagonal matrices,

$$\begin{pmatrix} a_1 & \bar{b}_1 & 0 & 0 & \cdots & 0 & 0 & \cdots \\ b_1 & a_2 & \bar{b}_2 & 0 & \cdots & 0 & 0 & \cdots \\ 0 & b_2 & a_3 & \bar{b}_3 & & \vdots & \vdots & \\ 0 & 0 & b_3 & a_4 & \ddots & & \vdots & \\ \vdots & \vdots & & \ddots & \ddots & \ddots & & \\ 0 & 0 & \cdots & & \ddots & a_n & \bar{b}_n & \\ 0 & 0 & \cdots & \cdots & & b_n & a_{n+1} & \ddots \\ \vdots & \vdots & & & & & \ddots & \ddots \end{pmatrix} \quad (1.1)$$

($b_i \in \mathbb{C}$, $a_i \in \mathbb{R}$) arise in the theory of moments,^{1,2} in noncommutative geometry,³⁻⁶ and in mathematical physics.⁷⁻¹¹ Such matrices clearly define symmetric operators S in the Hilbert space $\mathcal{H} = \ell^2$, and it can be checked that the corresponding deficiency indices (see (1.7) below) must be $(0,0)$ or $(1,1)$. These cases correspond to classical *limit-point*, respectively *limit-circle*, configurations for the corresponding generalized resolvent operators (see Refs. 12,13). The limit-point case yields a selfadjoint closure \bar{S} , and we say that S is *essentially selfadjoint*. This means that it has a spectral resolution which is given by the spectral theorem applied to \bar{S} . In the other case, there are nonzero vectors x_\pm in ℓ^2 such that

$$\langle x_\pm, Sy \pm iy \rangle_{\ell^2} = 0 \quad \text{for all finite sequences } y. \quad (1.2)$$

It is also known¹ that \bar{S} is selfadjoint if and only if $\sum_n |b_n|^{-1} = \infty$, assuming that the numbers b_n are all nonzero. (If some are zero, there is a natural modified condition.)

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The most basic example of such infinite tridiagonal matrices from quantum mechanics included the variables p, q from Heisenberg's $pq - qp = \frac{1}{\sqrt{-1}}I$. To see this, realize ℓ^2 as $L^2(\mathbb{R})$ via the orthonormal basis in $L^2(\mathbb{R})$ consisting of the Hermite functions $h_n(\cdot)$. Then $pf(x) = \frac{1}{\sqrt{-1}}f'(x)$ and $qf(x) = xf(x)$, say for f in the Schwartz space $\mathcal{S}(\mathbb{R})$, and the corresponding raising and lowering operators are $(p + iq)h_n = \sqrt{n+1}h_{n+1}$, and $(p - iq)h_n = \sqrt{n}h_{n-1}$, for $n = 0, 1, 2, \dots$. As a result, the respective matrices for p and q are as follows:

$$\frac{1}{2} \begin{pmatrix} 0 & 1 & & & & 0 \\ 1 & 0 & \sqrt{2} & & & \\ & \sqrt{2} & 0 & \sqrt{3} & & \\ & & \sqrt{3} & 0 & \ddots & \\ & & & \ddots & \ddots & \ddots \\ 0 & & & & \ddots & 0 & \sqrt{n} \\ & & & & & \sqrt{n} & 0 & \ddots \\ & & & & & & \ddots & \ddots \end{pmatrix}$$

and

$$\frac{1}{2\sqrt{-1}} \begin{pmatrix} 0 & -1 & & & & 0 \\ 1 & 0 & -\sqrt{2} & & & \\ & \sqrt{2} & 0 & -\sqrt{3} & & \\ & & \sqrt{3} & 0 & \ddots & \\ & & & \ddots & \ddots & \ddots \\ 0 & & & & \ddots & 0 & -\sqrt{n} \\ & & & & & \sqrt{n} & 0 & \ddots \\ & & & & & & \ddots & \ddots \end{pmatrix}.$$

One reason for the more general formulation (1.5) below, which is based on an increasing resolution of orthogonal projections, as opposed to an orthonormal basis, is that techniques which are effective in the simplest case of tridiagonal matrices carry over to the case when some symmetric operator S is formed by taking noncommuting functions of the p, q variables. Some such functions S are known to be essentially selfadjoint, and others not: for example, every quadratic expression S_2 in p, q which is symmetric is essentially selfadjoint, while $S_3 = pqp$ is not. Also $S_4 = p^2 - q^4$ is not essentially selfadjoint, but $p^2 + q^4$ is. These questions are also appropriate when we have instead an infinite number of degrees of freedom, i.e., infinite systems $\{p_i, q_j\}$; see, e.g., Refs. 6, 14.

In yet other applications, an orthonormal basis may not be readily available, while a resolution of projections $\{P_n\}$ may be. For example, such a resolution may come from a wavelet construction: in this case, usually such a resolution of projections is given at the outset, while the wavelet basis is technically much more complicated.

This classical setup from (1.1) serves as motivation for the results in the present paper. We now formulate a related geometric Hilbert space problem which turns out to generalize the one above, and which, as noted in Refs. 9–11, 15 and above, has many more applications.

Definition I.1 An operator S with dense domain $\mathcal{D}(S)$ in a Hilbert space \mathcal{H} is said to be *symmetric* (or Hermitian) if

$$\langle Sx, y \rangle = \langle x, Sy \rangle \quad \text{for all } x, y \in \mathcal{D}(S). \quad (1.3)$$

In terms of the adjoint operator S^* , this means that $S \subset S^*$, or equivalently, the domain of S is contained in that of S^* , and $Sx = S^*x$ for $x \in \mathcal{D}(S)$.

It was proved by von Neumann¹⁶ that the closure \bar{S} is selfadjoint in \mathcal{H} if and only if both of the *deficiency spaces*

$$\mathcal{E}_{\pm}(S) = \{x_{\pm} \in \mathcal{D}(S^*) ; S^*x_{\pm} = \pm ix_{\pm}\} \quad (1.4)$$

are zero. We say that a symmetric operator S is *smooth* if there is a sequence of projections

$$P_1 \leq P_2 \leq \dots \quad (1.5)$$

such that $P_j \mathcal{H} \subset \mathcal{D}(S)$, and $\bigcup_j P_j \mathcal{H}$ is dense in \mathcal{H} . The last density condition may be restated as

$$\sup_j P_j = I \quad (1.6)$$

where I denotes the identity operator in \mathcal{H} . As noted by Stone,¹² if S has dense domain, such projections P_j may always be constructed: we may even construct some smooth $\{P_j\}$ which has each P_j finite-dimensional, and for a given choice, there may be others which have better estimates on the corresponding off-diagonal terms. It is clear that the setting of smooth symmetric operators generalizes the classical matrix problem from (1.1). But for the more general operators, the *deficiency indices*

$$n_{\pm} := \dim \mathcal{E}_{\pm}(S) \quad (1.7)$$

need not be equal, and they may be more than one on either side, or infinite. For examples of this, see Ref. 11. Recall that it is known¹⁶ that S has selfadjoint extensions in \mathcal{H} if and only if $n_+ = n_-$.

If P_j is a sequence of projections associated to a given symmetric operator S , it is then clear from the geometric and general formulation that the operators $(I - P_j)SP_j$ may be viewed as off-diagonal terms, in a sense which naturally generalizes the off-diagonal terms b_j from the matrix (1.1) above. This is so since

$$P_j^{\perp} := I - P_j \quad (1.8)$$

is the projection onto the orthogonal complement of $P_j \mathcal{H}$. In an earlier paper⁹ we used the operator norms $\|P_j^{\perp}SP_j\|$ as a measure for the off-diagonal terms, but as noted in Ref. 9 this is a rough measure, and in the general case, the best result of this kind amounts to the assertion that boundedness of $\|P_j^{\perp}SP_j\|$ (as $j \rightarrow \infty$) implies essential selfadjointness.

In this paper, we refine this result, by considering the vectors $P_j^{\perp}SP_jx$ rather than the *operator norms* $\|P_j^{\perp}SP_j\|$. For one thing, the corresponding “local results” (i.e., depending on vectors) are more precise, and, secondly, it is difficult in practice to compute operator norms. As noted in Sakai’s book,¹⁷ the quantity $\|P_j^{\perp}SP_jx\|$ represents surface energy in statistical mechanics models.

II. A BASIC ESTIMATE

Let S be a symmetric operator with dense domain $\mathcal{D} := \mathcal{D}(S)$ in a Hilbert space \mathcal{H} , and let

$$\mathcal{E} := \mathcal{E}_+(S) = \{x \in \mathcal{D}(S^*) ; S^*x = ix\}. \quad (2.1)$$

Lemma II.1 *Let P be a smooth projection, and set $P^{\perp} := I - P$. Then we have the estimate*

$$\|P^{\perp}SPx\| \|P^{\perp}x\| \geq \|Px\|^2 \quad (2.2)$$

for all $x \in \mathcal{E}$.

Proof. If $x \in \mathcal{E}$ is given, then $S^*x = ix$. Applying P to both sides, and taking inner products, we get

$$\langle Px, S^*x \rangle = i \|Px\|^2. \quad (2.3)$$

But $\langle Px, S^*x \rangle = \langle SPx, x \rangle = \langle PSPx, x \rangle + \langle P^{\perp}SPx, x \rangle = \langle SPx, Px \rangle + \langle P^{\perp}SPx, P^{\perp}x \rangle$, and $\langle SPx, Px \rangle = \overline{\langle SPx, Px \rangle} = \overline{\langle Px, SPx \rangle}$. Hence

$$\operatorname{Im} \langle P^{\perp}SPx, P^{\perp}x \rangle = \|Px\|^2. \quad (2.4)$$

Since $|\operatorname{Im} \langle P^{\perp}SPx, P^{\perp}x \rangle| \leq |\langle P^{\perp}SPx, P^{\perp}x \rangle| \leq \|P^{\perp}SPx\| \|P^{\perp}x\|$, the result of the lemma follows. \square

Since the projection P has its range contained in $\mathcal{D}(S)$, the operator SP is bounded even though S is typically unbounded. The norm of the operator $P^{\perp}SP$ is a rough measure of the defect from selfadjointness for the given symmetric operator S , and we have the following:

Corollary II.2 *Let P be a smooth projection, and let $x \in \mathcal{E}$ (the defect space for a given symmetric operator S). Then we have the estimate,*

$$\|P^\perp SP|_{\mathcal{E}}\| \|P^\perp x\| \geq \|Px\|. \quad (2.5)$$

Proof. The result follows from the lemma, and the observation

$$\|P^\perp SPx\| \leq \|P^\perp SP|_{\mathcal{E}}\| \|Px\|. \quad (2.6)$$

If this is substituted into (2.4), and the term $\|Px\|$ is divided out, (2.5) follows. \square

Corollary II.3 (Jorgensen¹⁰) *Let S be a symmetric operator, and let $\{P_i\}_{i=1}^\infty$ be a sequence of smooth projections such that $\sup_i P_i = I$. Then if*

$$\sup_i \|P_i^\perp SP_i\| < \infty, \quad (2.7)$$

then S is essentially selfadjoint.

Proof. Apply the estimate (2.7) to both of the deficiency spaces

$$\mathcal{E}_\pm = \{x_\pm \in \mathcal{D}(S^*) ; S^* x_\pm = \pm i x_\pm\}. \quad (2.8)$$

The boundedness of $\{\|P_j^\perp SP_j\|\}_{j=1}^\infty$ implies that

$$\lim_{j \rightarrow \infty} \|P_j^\perp SP_j\| \|P_j^\perp x_\pm\| = 0 \quad (2.9)$$

since $\|x_\pm\| = \lim_{j \rightarrow \infty} \|P_j x_\pm\|$, and $\|P_j^\perp x_\pm\|^2 = \|x_\pm\|^2 - \|P_j x_\pm\|^2 \rightarrow 0$. An application of (2.5) then yields $x_\pm = 0$. This applies for any vector x_\pm in either of the two deficiency spaces \mathcal{E}_\pm . Hence both of these spaces must vanish, and it follows that S is essentially selfadjoint by von Neumann's theorem; see, e.g., Ref. 16. \square

The conclusion is that nontrivial defect for the given symmetric operator S implies unboundedness of the sequence of norms from (2.7).

Corollary II.4 *Let S and $\{P_j\}_{j=1}^\infty$ be as in Corollary II.3, but assume further that*

$$(I - P_{j+1}) SP_j = 0 \quad \text{for all } j = 1, 2, \dots \quad (2.10)$$

Then, if one of the defect spaces \mathcal{E}_\pm is nonzero, it follows that every positive sequence b_j such that the estimates

$$\|P_j^\perp SP_j\| \leq b_j \quad (2.11)$$

hold will satisfy

$$\sum_{j=1}^\infty \frac{1}{b_j^2} < \infty. \quad (2.12)$$

Proof. Suppose for simplicity that $x \in \mathcal{E}_+$ and $x \neq 0$. Then the added restriction (2.10) placed on the projections may be incorporated into the argument as follows: From (2.4) we have

$$\text{Im} \langle P_j^\perp SP_j x, x \rangle = \|P_j x\|^2.$$

But

$$\langle P_j^\perp SP_j x, x \rangle = \langle P_j^\perp SP_j x, (P_{j+1} - P_j) x \rangle$$

if (2.10) is assumed. Hence

$$\|P_j x\|^2 \leq b_j \|P_j x\| \|P_{j+1} x - P_j x\|,$$

where the estimates (2.11) are used. Cancelling a $\|P_j x\|$ factor, we get

$$\|P_j x\| \leq b_j \left(\|P_{j+1} x\|^2 - \|P_j x\|^2 \right)^{1/2}.$$

Equivalently, with the estimates (2.11), we therefore get

$$b_j^2 \|(P_{j+1} - P_j) x\|^2 \geq \|P_j x\|^2$$

and

$$b_j^2 \|P_{j+1} x\|^2 \geq (1 + b_j^2) \|P_j x\|^2.$$

Hence

$$\|P_{k+j} x\|^2 \geq \prod_{s=j}^{k+k-1} \left(1 + \frac{1}{b_s^2} \right) \|P_j x\|^2.$$

If $x \neq 0$, then there is some j such that $P_j x \neq 0$ and so the product $\prod_{j \leq x < j+k} (1 + 1/b_s^2)$ converges as $k \rightarrow \infty$, which implies the finiteness of the sum (2.12), and the result follows. \square

The following result is stronger than the corollary:

Theorem II.5 *With the assumptions of Corollary II.4, and assuming further that one of the deficiency spaces \mathcal{E}_\pm is nonzero, we get $\sum_{j=1}^\infty b_j^{-1} < \infty$.*

Proof. As in the previous proof, let $x \in \mathcal{E}_+ \setminus \{0\}$. By virtue of (2.10) we have

$$\langle P_j^\perp S P_j x, x \rangle = \langle P_j^\perp S P_j (P_j - P_{j-1}) x, (P_{j+1} - P_j) x \rangle$$

and therefore

$$\|P_j x\|^2 \leq b_j \|(P_j - P_{j-1}) x\| \|(P_{j+1} - P_j) x\|.$$

Pick j such that $P_j x \neq 0$. We will show that the numbers (b_k) from (2.11) yield $(b_k^{-1})_{k>j} \in \ell^1$. Summing the previous estimate, we now get the following:

$$\begin{aligned} \|P_j x\|^2 \sum_{k=j}^n b_k^{-1} &\leq \left(\sum_{k=j}^n \|(P_k - P_{k-1}) x\|^2 \sum_{k=j+1}^{n+1} \|(P_k - P_{k-1}) x\|^2 \right)^{1/2} \\ &= \|(P_n - P_{j-1}) x\| \|(P_{n+1} - P_j) x\| \\ &\leq \|x\|^2, \end{aligned}$$

and the result follows. \square

III. LOCAL ESTIMATES

The norm estimates on $P_j^\perp S P_j$ in the previous section are rather rough in that they do not yield direct asymptotic properties of the sequences $P_j^\perp S P_j x$ for fixed vectors x , and we now turn to this question, beginning with a basic lemma:

Lemma III.1 *Let S be a symmetric operator as in Section II, and let x be a nonzero vector in one of the deficiency spaces (2.8). Then*

$$\lim_{j \rightarrow \infty} \|P_j^\perp S P_j x\| = \infty; \tag{3.1}$$

more specifically, $\|P_j x\| < \|x\|$ for all j , and

$$\|P_j^\perp S P_j x\| \geq \frac{\|P_j x\|^2}{\sqrt{\|x\|^2 - \|P_j x\|^2}}. \tag{3.2}$$

Proof. From (2.4) in Section II, we get

$$\|P_j^\perp SP_j x\| \|P_j^\perp x\| \geq \|P_j x\|^2. \quad (3.3)$$

Since $\|P_j^\perp x\| = \sqrt{\|x\|^2 - \|P_j x\|^2}$, the estimate (3.2) follows. The conclusion (3.1) is implied by the estimate since $\lim_{j \rightarrow \infty} \|P_j x\|^2 = \|x\|^2$ from the assumption (1.6) on the sequence P_j . We always have $\|P_j x\| \leq \|x\|$, but this inequality is sharp. For if $\|P_j x\| = \|x\|$, then $P_j x = x$, and this contradicts the fact

$$\mathcal{D}(S) \cap \mathcal{E}_\pm = \{0\}. \quad (3.4)$$

To see this, note that $P_j x \in \mathcal{D}(S)$ since P_j is smooth, and $x \in \mathcal{E}_+$ by assumption. The conclusion of the lemma follows. \square

We now turn to the more restrictive class of symmetric operators S considered in Corollary II.4: While we have the subspaces $\mathcal{D}_j = P_j \mathcal{H}$ contained in the domain of S for all j , the more restrictive assumption in Corollary II.4 is that S maps \mathcal{D}_j into the next space \mathcal{D}_{j+1} . Note that, if $\bigcup_j \mathcal{D}_j$ is mapped into itself, we can always arrange, by relabeling the indexing of the subspaces, that this condition is satisfied relative to the relabeled sequence of subspaces. This means that the corresponding projections P_j will then satisfy the property (2.10) from Corollary II.4. We now turn to the sequence $\|P_j^\perp SP_j x\|$ for the case when S has at least one nontrivial deficiency space, i.e., when one of the two spaces $\mathcal{E}_\pm(S)$ is assumed nonzero. We already showed in Lemma III.1 that then $\|P_j^\perp SP_j x\| \rightarrow \infty$ as $j \rightarrow \infty$, and so we may assume without loss of generality that the numbers $\|P_j^\perp SP_j x\|$ are all nonzero.

The next result specifies a growth rate for this sequence in case of nonzero deficiency. To apply the result in proving essential selfadjointness of some given symmetric operator S , with the scaling property (3.6), we can then check that the sequence $\|P_j^\perp SP_j x\|$ grows less rapidly than the *a priori* rate (see (3.8)) and S must then have selfadjoint closure.

Theorem III.2 *Let S be a densely defined symmetric operator which has a smooth sequence of projections P_j with*

$$\sup_j P_j = I \quad (3.5)$$

and

$$P_{j+1} SP_j = SP_j \quad \text{for all } j = 1, 2, \dots \quad (3.6)$$

Suppose one of the deficiency spaces is nonzero. Let $x \in \mathcal{E} \setminus \{0\}$. Then there is a number $\xi \in (0, 1)$, the open unit interval, such that the local sequence

$$c_j = c_j(x) := \|P_j^\perp SP_j x\|^2 \quad (3.7)$$

grows so rapidly as to yield existence of the limit

$$\lim_{j \rightarrow \infty} F_{c_{j+1}}(F_{c_j}(\dots(F_{c_2}(F_{c_1}(\xi)))\dots)) \leq 1, \quad (3.8)$$

where

$$F_c(s) = s + \frac{1}{c}s^2, \quad s \in \mathbb{R}_+. \quad (3.9)$$

Moreover, then $\sum_j 1/c_j < \infty$.

Proof. The start of the proof is the same as that of Corollary II.4, but then the next estimate is refined as follows: Suppose for specificity that $x \in \mathcal{E}_+$, and that $\|x\| = 1$. By virtue of the assumption on S , we have

$$\langle P_j^\perp SP_j x, x \rangle = \langle P_j^\perp SP_j x, (P_{j+1} - P_j)x \rangle \quad (3.10)$$

and

$$\operatorname{Im} \langle P_j^\perp SP_j x, x \rangle = \|P_j x\|^2.$$

As a consequence, we get the estimate

$$\|P_j x\|^2 \leq c_j^{1/2} \|P_{j+1} x - P_j x\|, \quad (3.11)$$

where the sequence c_j is defined in (3.7). Introducing $\xi_j := \|P_j x\|^2$, we note that $0 < \xi_j < 1$, and $\lim_{j \rightarrow \infty} \xi_j = 1$ ($= \|x\|^2$), and the limit is monotone. Also note that the functions F_c from (3.9) are monotone on \mathbb{R}_+ . Now the estimate (3.11) takes the form

$$\xi_j^2 \leq c_j (\xi_{j+1} - \xi_j), \quad (3.12)$$

or equivalently

$$F_{c_j}(\xi_j) \leq \xi_{j+1} \quad \text{for all } j = 1, 2, \dots \quad (3.13)$$

Starting with the initial estimate $F_{c_1}(\xi_1) \leq \xi_2$, and using monotonicity of F_{c_2} , we get

$$F_{c_2}(F_{c_1}(\xi_1)) \leq F_{c_2}(\xi_2) \leq \xi_3,$$

and then, by induction,

$$\underbrace{F_{c_j}(F_{c_{j-1}}(\dots(F_{c_2}(F_{c_1}(\xi_1)))\dots))}_{=: t_j} \leq \xi_{j+1}.$$

It also follows from (3.9) that the sequence t_j is monotone and strictly increasing. Indeed, $t_{j+1} = t_j + \frac{1}{c_{j+1}} t_j^2 > t_j$ for all j . Since $\xi_{j+1} = \|P_{j+1} x\|^2 < 1$, with limit $= 1$, the result follows. The last conclusion in the theorem will be proved in the next section. \square

Remark III.3 It follows from the theorem that if the containment $\bar{S} \subset S^*$ is strict, then there are vectors x in $\mathcal{D}(S^*)$ such that the boundary terms $c_n(x) = \|P_n^\perp S P_n x\|^2$ have growth asymptotics at least some *a priori* rate. If further (3.6) is assumed, then this rate may be specified as

$$\sum_n c_n(x)^{-1} < \infty. \quad (3.14)$$

But we have the following converse: Suppose, for some $x \in \mathcal{D}(S^*)$, that (3.14) holds. Then x cannot be in the domain of \bar{S} , and so $\bar{S} \subsetneq S^*$, or equivalently, S is then not essentially selfadjoint. This is strong enough for proving that the noncommutative polynomials pqp and $p^2 - q^4$ from Section I are not essentially selfadjoint on the span \mathcal{D} of the Hermite polynomials, and therefore *a fortiori* also not on \mathcal{S} .

To prove the claim, suppose a symmetric operator S is given to satisfy the conditions in Theorem III.2. We claim that, if $x \in \mathcal{D}(\bar{S})$, then $c_n(x) = \|P_n^\perp S P_n x\|^2$ is bounded. This clearly is inconsistent with (3.14), so if (3.14) holds for some $x \in \mathcal{D}(S^*)$, then \bar{S} is not selfadjoint. We now prove boundedness of $c_n(x)$ for $x \in \mathcal{D}(\bar{S})$: If $x \in \mathcal{D}(\bar{S})$, then $S P_n x \rightarrow \bar{S} x$, and so it is enough to prove boundedness if $x \in \mathcal{D} := \bigcup_n P_n \mathcal{H} (\subset \mathcal{D}(S))$. Let $x \in P_n \mathcal{H}$, i.e., $P_n x = x$. Then $P_j x = P_j P_n x = P_n x$ for all $j \geq n$, and, using (3.6), $P_j^\perp S P_j x = P_j^\perp S P_n x = P_j^\perp P_{n+1} S x = 0$ if $j \geq n+1$. Hence $c_j(x) = 0$ if $j \geq n+1$, and $\lim_{j \rightarrow \infty} c_j(x) = 0$ for all $x \in \mathcal{D}$. We leave the remaining approximation argument for the reader, i.e., passing to vectors x in $\mathcal{D}(\bar{S})$.

IV. FUNCTIONAL ITERATION

The condition (3.8) of Theorem III.2 is perhaps not as transparent as the corresponding condition (2.12) in Corollary II.4. But there is a simple comparison between the two sequences

$$b_j = \|P_j^\perp S P_j\| \quad \text{and} \quad c_j(x) = \|P_j^\perp S P_j x\|^2. \quad (4.1)$$

Clearly

$$c_j(x) \leq \|x\|^2 b_j^2. \quad (4.2)$$

So if x is a nonzero vector in one of the two deficiency spaces \mathcal{E}_\pm , then

$$\sum_j \frac{1}{b_j^2} \leq \|x\|^2 \sum_j \frac{1}{c_j(x)}. \quad (4.3)$$

The condition from Corollary II.4 is (2.12), and its negation,

$$\sum_j \frac{1}{b_j^2} = \infty, \quad (4.4)$$

implies selfadjointness. We conclude then that if x is any nonzero vector, then the condition

$$\sum_j \frac{1}{c_j(x)} = \infty \quad (4.5)$$

follows from (4.4). We now show that Theorem III.2 is strictly stronger than Corollary II.4. To this end we state a simple lemma on functional iteration which explains the two types of estimates involved.

Lemma IV.1 *Let $\{c_j\}_{j=1}^\infty \subset \mathbb{R}_+$ be given. Then the following two conditions are equivalent:*

1. $\sum_j 1/c_j < \infty$;
2. *There is a $\xi \in (0, 1)$ such that*

$$F_{c_j}(F_{c_{j-1}}(\cdots(F_{c_2}(F_{c_1}(\xi)))\cdots)) < 1 \quad \text{for all } j = 1, 2, \dots \quad (4.6)$$

Proof. (1) \Rightarrow (2): Assume (1). Since $\ln(1 + 1/c_i) < 1/c_i$, we get $\ln \prod_{i=1}^j (1 + 1/c_i) < \sum_{i=1}^j 1/c_i$, the infinite product then converges, and $\prod_{i=1}^\infty (1 + 1/c_i) < \exp(\sum_{i=1}^\infty 1/c_i) < \infty$. Hence we may pick $\xi \in (0, 1)$ such that

$$\prod_{i=1}^j \left(1 + \frac{1}{c_i}\right) \xi < \prod_{i=1}^\infty \left(1 + \frac{1}{c_i}\right) \xi < 1 \quad \text{for all } j. \quad (4.7)$$

If we prove that

$$t_j := F_{c_j}(F_{c_{j-1}}(\cdots(F_{c_1}(\xi)))\cdots) < \prod_{i=1}^j \left(1 + \frac{1}{c_i}\right) \xi, \quad (4.8)$$

then the first implication of the lemma follows. But this is an induction argument: Suppose it holds up to $j - 1$. Then by (4.7), we will have $t_{j-1} = F_{c_{j-1}}(F_{c_{j-2}}(\cdots(F_{c_1}(\xi)))\cdots) < 1$, and therefore, using $t_{j-1}^2 < t_{j-1}$, we get

$$t_j = F_{c_j}(t_{j-1}) = t_{j-1} + \frac{1}{c_j} t_{j-1}^2 < \left(1 + \frac{1}{c_j}\right) t_{j-1} < \prod_{i=1}^j \left(1 + \frac{1}{c_i}\right) \xi,$$

where, in the last step, the induction hypothesis was used a second time. This concludes the induction step, and (4.8) is proved. By the choice of ξ in (4.7), we now get the desired conclusion (4.6) of the lemma. \square

(2) \Rightarrow (1): Assume (2). The first two estimates in (4.6) are

$$t_1 = \xi + \frac{1}{c_1} \xi^2 < 1,$$

and

$$t_2 = \xi + \frac{1}{c_1} \xi^2 + \frac{1}{c_2} \left(\xi + \frac{1}{c_1} \xi^2\right)^2 < 1.$$

Completing the second square, we get five positive terms in the sum on the left, and so *a fortiori*

$$\frac{1}{c_1} \xi^2 + \frac{1}{c_2} \xi^2 < 1$$

when only two out of the five terms are retained in the sum. But the general term

$$t_j = F_{c_j} (F_{c_{j-1}} (\cdots (F_{c_2} (F_{c_1} (\xi))) \cdots))$$

on the left-hand side in (4.6) includes, when all the squares are completed, the following j terms:

$$\frac{1}{c_1} \xi^2 + \frac{1}{c_2} \xi^2 + \cdots + \frac{1}{c_j} \xi^2 \quad (< t_j)$$

among a total of $3 \cdot (j-1)$ positive terms. Since all these terms sum up to $t_j < 1$, we get, for the retained ones, $(\sum_{i=1}^j 1/c_i) \xi^2 < t_j < 1$, and therefore $\sum_{i=1}^\infty 1/c_i < \infty$. \square

Proposition IV.2 *The implication in Corollary II.4 may be derived from that of Theorem III.2, and Theorem III.2 applies to cases not covered by Corollary II.4.*

Proof. Suppose $x \in \mathcal{E}(S) \setminus \{0\}$. Normalize such that $\|x\| = 1$. Then, by Theorem III.2, we may pick j such that $\xi = \|P_j x\|^2 \in (0, 1)$ will satisfy $F_{c_{j+k}} (F_{c_{j+k-1}} (\cdots (F_{c_{j+1}} (\xi)) \cdots)) < 1$ for all k . Using the lemma, we get $\sum_j 1/c_j < \infty$, and by (4.3), we must then have $\sum_j 1/b_j^2 < \infty$. This shows that Theorem III.2 is the stronger of the two results. The examples in Ref. 11 further show that, in fact, the result in Section III is strictly stronger than that of Section II. \square

V. POSITIVE OPERATORS

We say that a symmetric operator L with dense domain in a Hilbert space \mathcal{H} is positive if

$$\langle y, Ly \rangle \geq 0, \quad y \in \mathcal{D}(L). \quad (5.1)$$

For vectors $x \in \mathcal{H}$, then the sequence

$$d_n(x) := \langle x, P_n^\perp L P_n x \rangle, \quad n \in \mathbb{N}, \quad (5.2)$$

is a more natural measure for off-diagonal terms, relative to some system $\{P_n\}_{n=1}^\infty$ of smooth projections with $\sup_n P_n = I$; and we have the following obvious estimate:

$$d_n(x) \leq c_n(x)^{1/2} \|x\|, \quad (5.3)$$

where $c_n(x) = c_n(L, x) := \|P_n^\perp L P_n x\|^2$. As a result, we have the following estimate for the sums

$$\sum_n c_n(x)^{-1/2} \leq \|x\| \sum_n d_n(x)^{-1} \quad (5.4)$$

for all nonzero vectors x in \mathcal{H} . Hence, if a given symmetric operator L is also known to be positive, then we get the following improvement on Theorem III.2.

Theorem V.1 *Let L be a positive operator, and suppose $\{P_n\}_{n=1}^\infty$ are smooth projections satisfying*

$$\sup_n P_n = I, \quad (5.5)$$

and suppose further, for some $k \in \mathbb{N}$, that

$$P_{n+k} L P_n = L P_n \quad \text{for all } n. \quad (5.6)$$

If $x \in \mathcal{E}_\pm(L) \setminus \{0\}$, then $\sum_n c_n(x)^{-1/2} < \infty$.

Proof. The result in fact is a consequence of the following more general one, combined with (5.4). \square

Theorem V.2 *Let L be a positive operator, and let $\{P_n\}_{n=1}^\infty$ be smooth projections satisfying (5.5)–(5.6). Then, if $x \in \mathcal{D}(L^*) \setminus \{0\}$ satisfies $L^*x = -x$, we get the summability:*

$$\sum_n d_n(x)^{-1} < \infty. \quad (5.7)$$

Proof. This result is implicit in the proof of Lemma 1 in Ref.¹⁸. We will also need the general fact¹⁶ that positive operators L with dense domain are essentially selfadjoint if and only if $\{x \in \mathcal{D}(L^*) ; L^*x = -x\} = \{0\}$. \square

Let $\{S_i\}_{i=1}^k$ be a finite family of symmetric operators in a Hilbert space \mathcal{H} which are defined on a common dense invariant domain \mathcal{D} in \mathcal{H} . Then $L := \sum_{i=1}^k S_i^2$ is positive and defined on \mathcal{D} . Nelson¹⁹ and Poulsen²⁰ studied the question of deciding when the operators S_i are selfadjoint with commuting spectral resolutions. A necessary condition for this is the commutativity

$$S_i S_j y = S_j S_i y \quad \text{for all } i, j \leq k, \text{ and all } y \in \mathcal{D}. \quad (5.8)$$

If such commuting spectral resolutions exist, then there is, by Refs. 16,13, a spectral measure $E(\cdot)$ on \mathbb{R}^k such that

$$S_i x = \int_{\mathbb{R}^k} \lambda_i dE(\lambda) x \quad (5.9)$$

and

$$\|x\|^2 = \int_{\mathbb{R}^k} \|dE(\lambda) x\|^2, \quad (5.10)$$

where we use the standard notation $\mathbb{R}^k \ni \lambda = (\lambda_1, \dots, \lambda_k)$.

Nelson's celebrated theorem (see also Ref. 20) states that a joint spectral resolution (5.9) exists if the S_i 's satisfy (5.8), and if $L = \sum_i S_i^2$ is essentially selfadjoint on \mathcal{D} .

Our off-diagonal terms from Theorem III.2 are especially useful in the multivariable case, as is illustrated in the following theorem.

Theorem V.3 *Let $\{S_i\}_{i=1}^k$ be given symmetric operators satisfying (5.8). Let $\{P_n\}_{n=1}^\infty$ be smooth projections such that $P_n \mathcal{H} \subset \mathcal{D}$, $\sup_n P_n = I$, and*

$$P_{n+1} S_i P_n = S_i P_n \quad \text{for all } 1 \leq i \leq k, \text{ and all } n \in \mathbb{N}, \quad (5.11)$$

i.e., each S_i satisfying the conditions in Theorem III.2. Suppose, for all $x \in \mathcal{H}$, that we have the following asymptotics:

$$c_i(n, x) = \|P_n^\perp S_i P_n x\|^2 \leq \mathcal{O}(n). \quad (5.12)$$

Then the closed operators \bar{S}_i are selfadjoint (the S_i 's are essentially selfadjoint on \mathcal{D}), and they have joint spectral resolution in the sense of (5.9).

Proof. For Nelson's operator $L = \sum_{i=1}^k S_i^2$, we have off-diagonal defect terms as follows:

$$\begin{aligned} d(L, n, x) &= \langle P_n^\perp L P_n x, x \rangle \\ &= \langle L(P_n - P_{n-2})x, (P_{n+2} - P_n)x \rangle \\ &= \sum_i \langle S_i(P_n - P_{n-2})x, S_i(P_{n+2} - P_n)x \rangle \\ &= \sum_i \langle P_{n-1}^\perp S_i P_n x, P_{n+1}^\perp S_i P_{n+2} x \rangle \\ &= \sum_i \langle P_{n+1}^\perp S_i P_n x, P_{n+1}^\perp S_i P_{n+2} x \rangle \\ &= \sum_i \langle P_{n+1}^\perp P_n^\perp S_i P_n x, P_{n+1}^\perp S_i P_{n+1} x \rangle \\ &\leq \sum_i \|P_n^\perp S_i P_n x\| \|P_{n+1}^\perp S_i P_{n+1} x\| \\ &\leq \left(\sum_{i=1}^k c_i(n, x) \sum_{j=1}^k c_j(n+1, x) \right)^{1/2} \\ &\leq \mathcal{O}(n) \end{aligned}$$

by virtue of the assumption (5.12) made for each of the operators S_i . Each S_i is essentially selfadjoint on \mathcal{D} by Theorem III.2; but *a priori* the corresponding spectral resolutions $E_i(\cdot)$ may not commute (see, e.g., Refs. 19, 21, or 22,23). However, since $d(L, n, x) \leq \mathcal{O}(n)$ for all $x \in \mathcal{H}$, we conclude from Theorem V.2 above that $L = \sum_{i=1}^k S_i^2$ is then essentially selfadjoint on \mathcal{D} . Hence, Nelson's theorem¹⁹ implies that the individual spectral resolutions $E_i(\cdot)$ on \mathbb{R} are mutually commuting. So, if we define E on \mathbb{R}^k as a product measure, $dE(\lambda) = E_1(d\lambda_1) E_2(d\lambda_2) \cdots E_k(d\lambda_k)$, then it follows from standard spectral theory (see, e.g., Ref. 16) that $E(\cdot)$ (on \mathbb{R}^k) will satisfy (5.9)–(5.10). \square

Remark V.4 The multivariable case in the present section is especially useful in recent work on multivariable spectral theory by Vasilescu et al.^{21,24} There, in applications to multivariable moment problems, the issue of commutativity of symmetric operators in the weak sense, versus the strong sense, is related to comparison of joint distributions vs. marginal distributions.

Other applications to mathematical physics are sketched in Refs. 23 and 9–11,18,25. In particular, our assumptions are especially useful in the study of noncommutative polynomials applied to quantum fields like momentum and position bosonic variables, as they are given traditionally in terms of raising and lowering operators.

A simple application of Theorem V.2 then yields the following concrete corollary: Let

$$(p_i h)(x) = \frac{1}{\sqrt{-1}} \frac{\partial}{\partial x_i}(x),$$

and

$$(q_j h)(x) = x_j h(x_1, \dots, x_k)$$

for $h \in \mathcal{S}(\mathbb{R}^k) \subset L^2(\mathbb{R}^k)$. Let L be a noncommutative polynomial in the variables p_i, q_j for $1 \leq i, j \leq k$ of degree at most four, such that $\langle h, Lh \rangle_{L^2(\mathbb{R}^k)} \geq 0$ for all $h \in \mathcal{S}(\mathbb{R}^k)$. Then it follows that L is essentially selfadjoint on $\mathcal{S}(\mathbb{R}^k) \subset L^2(\mathbb{R}^k)$, and the spectrum of \bar{L} is positive.

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